Unique Linear Solver Needs of the Los Alamos Radiation Transport Team

Michael L. Hall
John M. McGhee
Group CIC-19, Radiation Transport Team
P.O. Box 1663, MS-B265
Los Alamos National Laboratory
Los Alamos, New Mexico 87545 USA
Email: **hall@lanl.gov**

8 / 28 / 96

Outline

- DANTE
  - Problem Characteristics
  - Matrix Characteristics
  - Matrix Storage
  - Current Solution
- Augustus / Spartan
  - Problem Characteristics
  - Matrix Characteristics
  - Discretization
  - Current Solution
- Overall Needs of Radiation Transport

DANTE

Problem Characteristics

- Radiation Transport (S_N, SP_N, P_N)
- 1–D, 2–D, 3–D Cartesian
- Arbitrary Finite Element (Hexahedra, Tetrahedra, etc.)
- Unstructured Mesh — Node-Based
- Variables: Intensity for every point, angle and energy group (energy groups always decouple)

DANTE

Matrix Characteristics

- Size (rows): S_N & SP_N: n_{nodes};
  P_N: $n_{nodes} \times F\left(n_{angles}\right)$
- Absolute size (rows): 10,000 – 1,000,000
- Sparse ($\approx$ 10 non-zeroes per row)
- Actual number of non-zeroes per row unknown
- Symmetric Positive Definite
- P_N: full block matrix, each block has same non-zero pattern
- S_N & SP_N: block diagonal matrix (angles uncouple)

DANTE

System Storage

- Multi-D Vectors: `v(npoints, nangles)`
- Matrix: complicated, never assembled
- Reverse communication necessary
- Some treatment of dot products necessary

DANTE

Current Solution

- Conjugate Gradient with Jacobi preconditioning
  (developed in-house)

- Algebraic Unstructured Multigrid
  (Mantueffel et al., experimental)

- Would like to be able to use standard preconditioners with
  reverse communication

Augustus / Spartan
Problem Characteristics

- Radiation Transport (SPARTAN: SP_N, AUGUSTUS: P_1)
- AUGUSTUS: 1–D (Cartesian, Cylindrical & Spherical), 2–D (Cartesian & Cylindrical), 3–D (Cartesian)
- SPARTAN: 2–D (Cartesian & Cylindrical)
- SPARTAN uses AUGUSTUS as its solver, so multi–D version of SPARTAN is on the way
- 3–D: Hexahedra & Degenerates,
  2–D: Quadrilaterals & Degenerates,
  1–D: Line Segments
- Unstructured Mesh
- SPARTAN Variables: Intensity for every point, angle and energy group (energy groups and angles always decouple)

Augustus / Spartan
Matrix Characteristics

Main Matrix System:

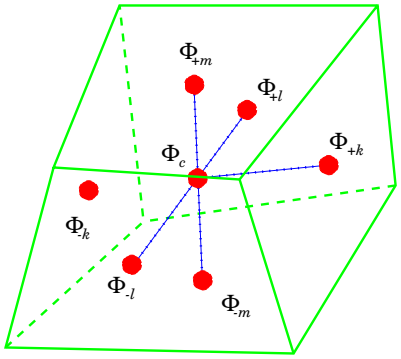
- Size (rows): $4\ n_{cells} + n_{bf}/2$
- Absolute size (rows): 10,000 – 100,000
- Sparse (7 or 11 non-zeroes per row)
- Unsymmetric
- ELL Storage

Preconditioner Matrix System:

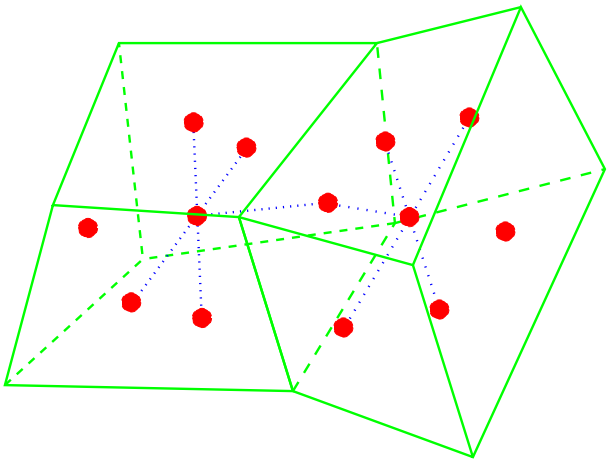
- Size (rows): n_{cells}
- Sparse (7 non-zeroes per row)
- Symmetric
- ELL Storage

Augustus / Spartan Discretization

Main system involves cell-equations ($+k$ flux shown, all points would be involved in cell-equation):



and cell-face equations:



Preconditioner eliminates minor directions in flux terms to yield a system involving only cell-centers.

Augustus / Spartan
Current Solution

Main system:

- Krylov space solvers (GMRES, BCGS, etc.) in JTPACK by John Turner, LANL
- UMFPACK: incomplete direct method (the unstructured multi-frontal method) by Tim Davis, U of FL

Preconditioner:

- Jacobi, SSOR, ILU from JTPACK
- Specialized Low-Order Preconditioner, solved with Conjugate Gradient with SSOR preconditioning using JTPACK
- UMFPACK: none

Overall Needs of Radiation Transport

- JTPACK, UMFPACK serving most needs
- Would like to be able to use standard preconditioners with reverse communication
- Reverse communication for matrix multiplication and system solution (possibly for dot products)
- Support for 2–D vectors
- Arithmetic Unstructured Multigrid Package with Documentation

Implementation:
The Augustus Code Package

Author:	Michael L. Hall (1/94 - present)
Architectures:	Sun (SunOS and Solaris), SGI (IRIX), HP (HP-UX), IBM (AIX)
Language:	Fortran-77, plans for Fortran-90
Solver Packages:	JTPACK (by John Turner, LANL) for Krylov Space methods, UMFPACK (by Tim Davis, U of FL) for sparse direct methods
Installations:	SNLA ALEGRA hydrodynamics code, LANL TELLURIDE low-speed flow code, Solver for the SPARTAN SP_N radiation transport code.
Status:	Completed, active development of new features
Availability:	Email **hall@lanl.gov** and we'll talk